Powertrain Core Program: High-Temperature Aluminum Alloys

2019 DOE Vehicle Technologies Office Annual Merit Review Presentation

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June 13, 2019 Project ID#mat159

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Program Overview

Timeline

- Lab call award: Jul 2018
- Program start: Oct 2018
- End: Sept 2023
- 5% Complete

Budget

- New Powertrain Materials Core Program (PMCP):
  - $30M / 5 years

FY19 PMCP Research Thrusts	FY19 Budget
1. Cost Effective LW High Temp Engine Alloys	$1.15M
2. Cost Effective Higher Temp Engine Alloys	$1.55M
3. Additive Manufacturing of Powertrain Alloys	$1.05M
4. Advanced Characterization & Computation	$1.55M
5. Emerging Technologies	$0.7M

Barriers

- Higher power density engines resulting in more extreme materials demands
- Cost of advanced materials
- Development time/cost of new materials
- Scaling new materials technologies to commercialization

Partners

- Program Lead
  - Oak Ridge National Lab (ORNL)
- Program Partners
  - Pacific Northwest National Lab (PNNL)
  - Argonne National Lab (ANL)

Thrust 1/Subtask 1A1 Overview

1A1. Fundamental studies of complex precipitation pathways

Timeline

- Project start: Oct 2018
- End: Sept 2023
- 5% Complete

Budget

- **Thrust 1 total:** $1.15M (DOE funds)

FY19 Thrust 1 Tasks	FY19 Budget
1. Cost Effective LW High Temp Engine Alloys	
1A1. Fundamental studies of precipitation pathways	$0.35M
1A2. New higher performance Al alloys ($\geq$400^{o}C)	$0.4M
1B1. Intermediate Temp ACMZ Alloys	$0.3M
1B2. Tailored ACMZ Alloys	$0.1M

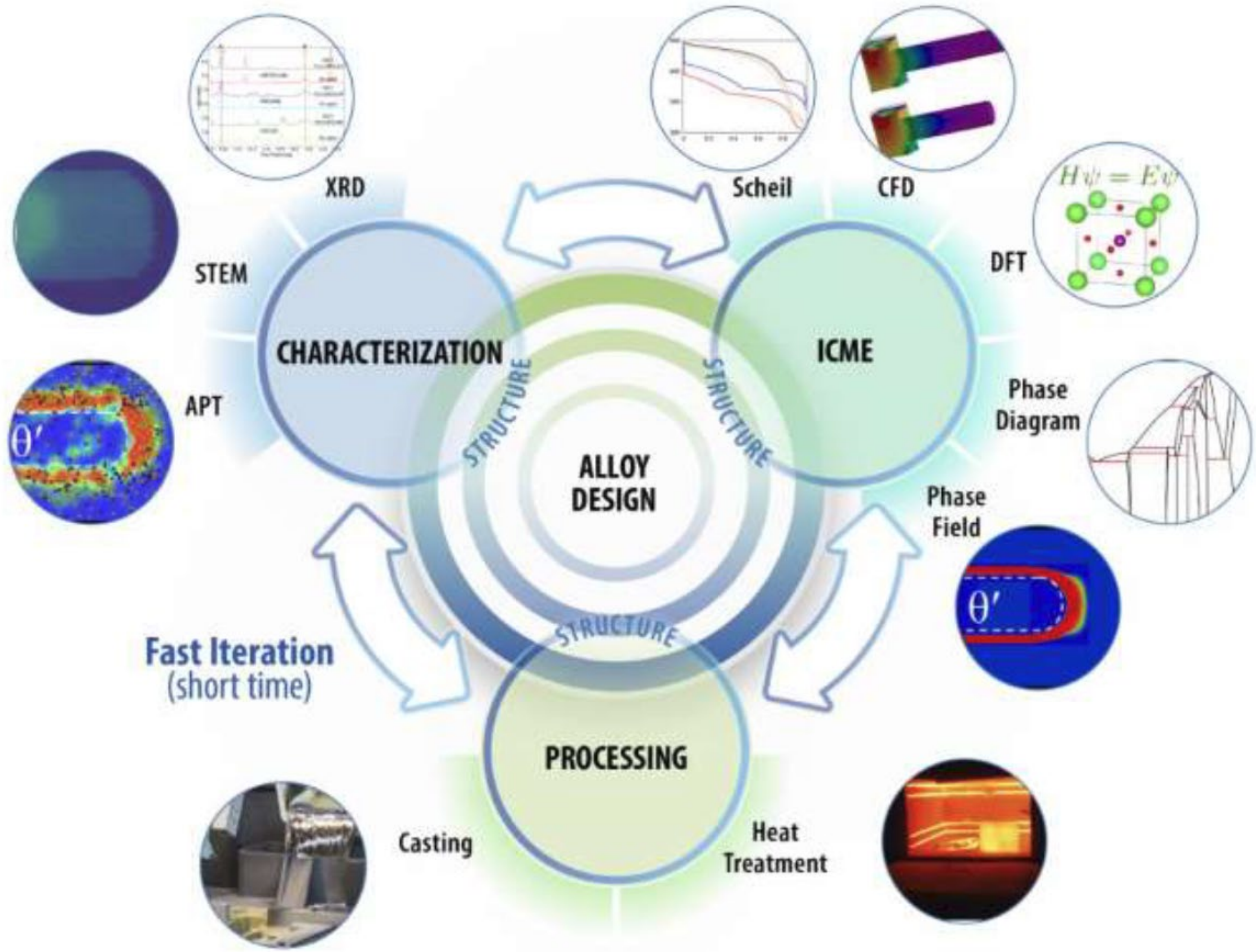
Barriers

- Materials performance and cost constrain design of future advanced powertrains that achieve increased efficiency, lower emissions, improved performance and light weight (LW) structures; while also maintaining reliability and durability.
- Development time. Project leverages an ***Integrated computational materials engineering*** (ICME) framework to reduce the early & mid-stage development time of new LW alloys by 50%.

Partners

- Thrust 1 lead
  - Oak Ridge National Lab (ORNL)
- Partners
  - Pacific Northwest National Lab (PNNL)
  - Argonne National Lab (ANL)

Relevance – Thrust Objective



- Develop, using ICME, higher temperature lightweight engine materials with improved strength and thermal stability, leading to further increases in power densities of engines.

Milestones

Thrust milestones in FY19

- Q1) Finish assessment of high temperature aluminum alloy systems (>400^{o}C) for further research - **completed**
- Q2) Submit joint experimental and theory publication on co-precipitates with high temperature stability – on track
- Q3) Initiate CRADA discussion on intermediate temperature ACMZ alloys – on track
- Q4) Complete neutron diffraction analysis of mechanical behavior for one aluminum alloy – on track

Approach

Alloy development – chemistry and heat treatment

 # Topic 1

Atomistic behavior of interfaces

 # Topic 2

Microstructural Evolution

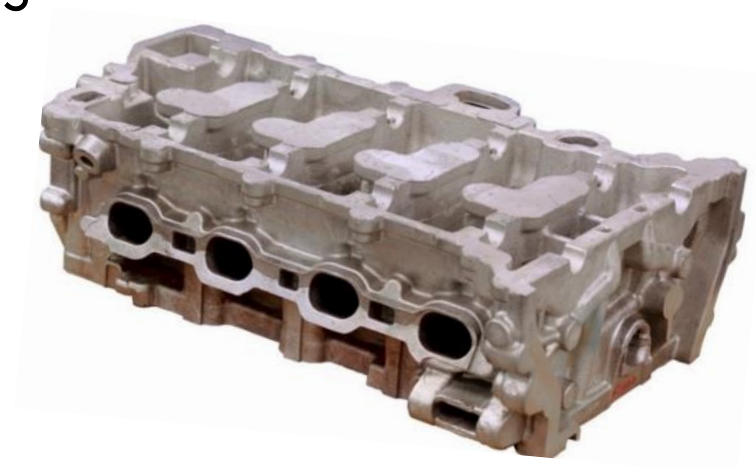
 # Topic 3

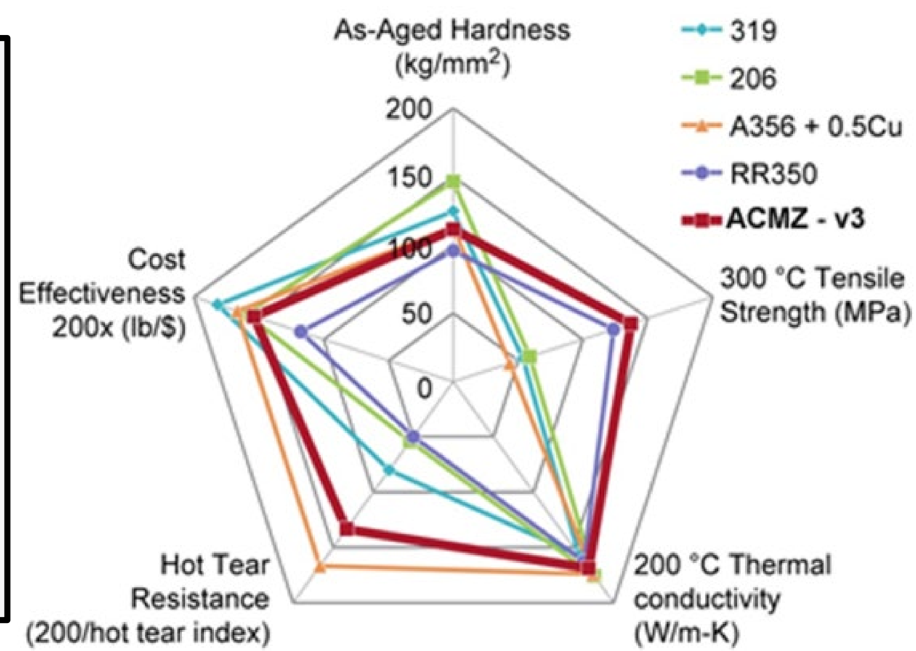
(Mechanical) Property Prediction

- Primary focus is higher temperature (up to 400°C) cast aluminum alloys for powertrain applications (cylinder head, piston, turbocharger etc.).
- Linking experiments with simulations emphasized
- Target properties are set to address technical gaps. Co-operative research agreements with industry will validate effectiveness of targets.

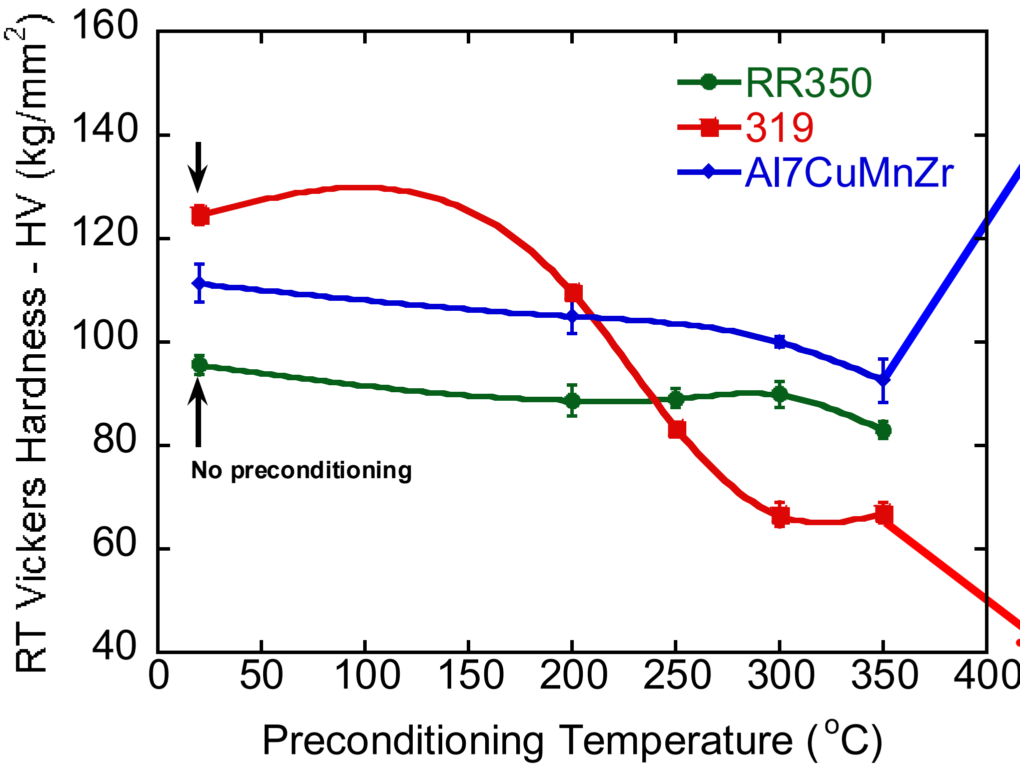
Cast AlCuMnZr (ACMZ) alloys

- VTO FOA Award led to 4 year CRADA with industry
- ICME played a key role
- Team and DOE recognition of applying the approach to a broad range of needs

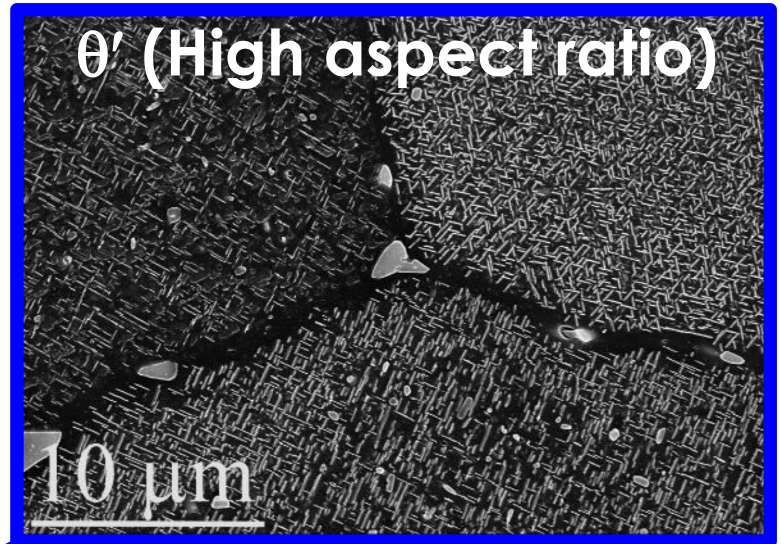




Hardness change due to prolonged elevated temperature exposure – Comparison between <u>ACMZ</u> and conventional alloys



Al7CuMnZr



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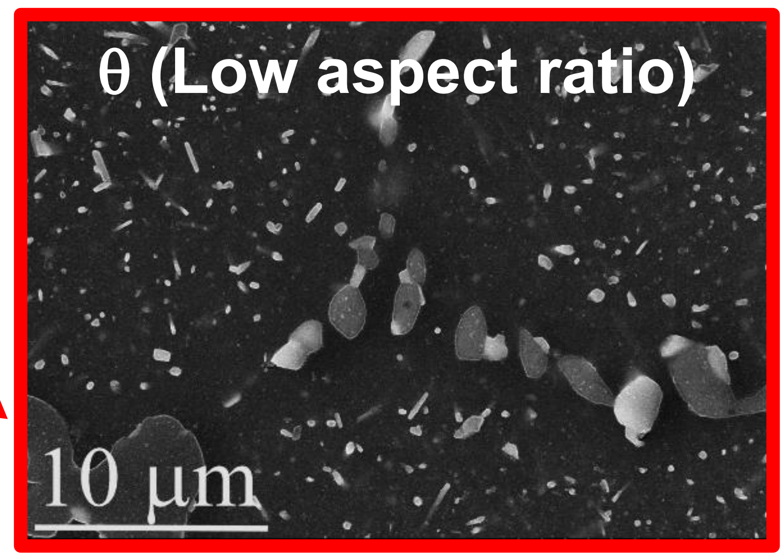
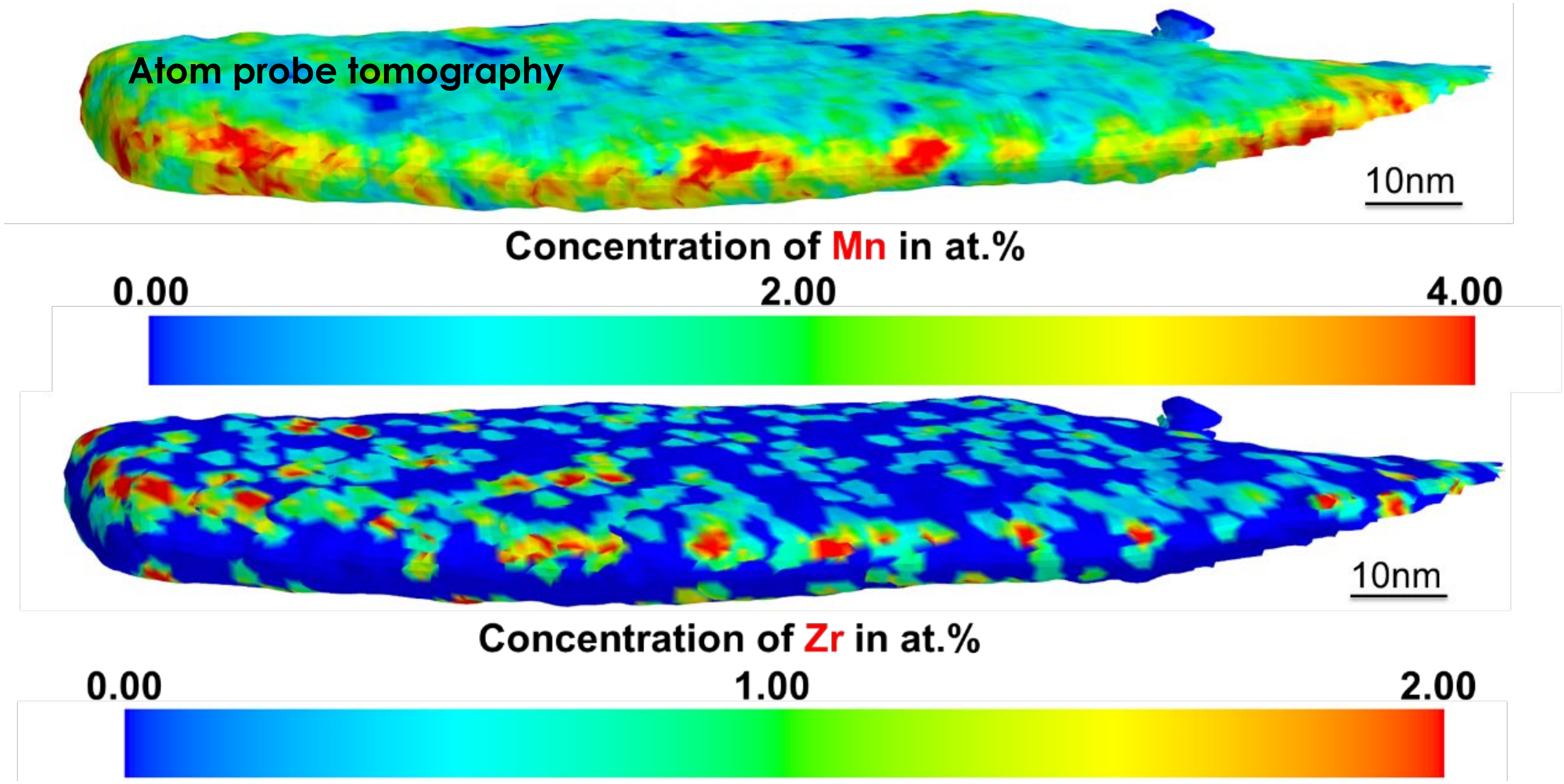


Solute segregation to interfaces of θ′ precipitate determines the thermal stability of Al-Cu alloys

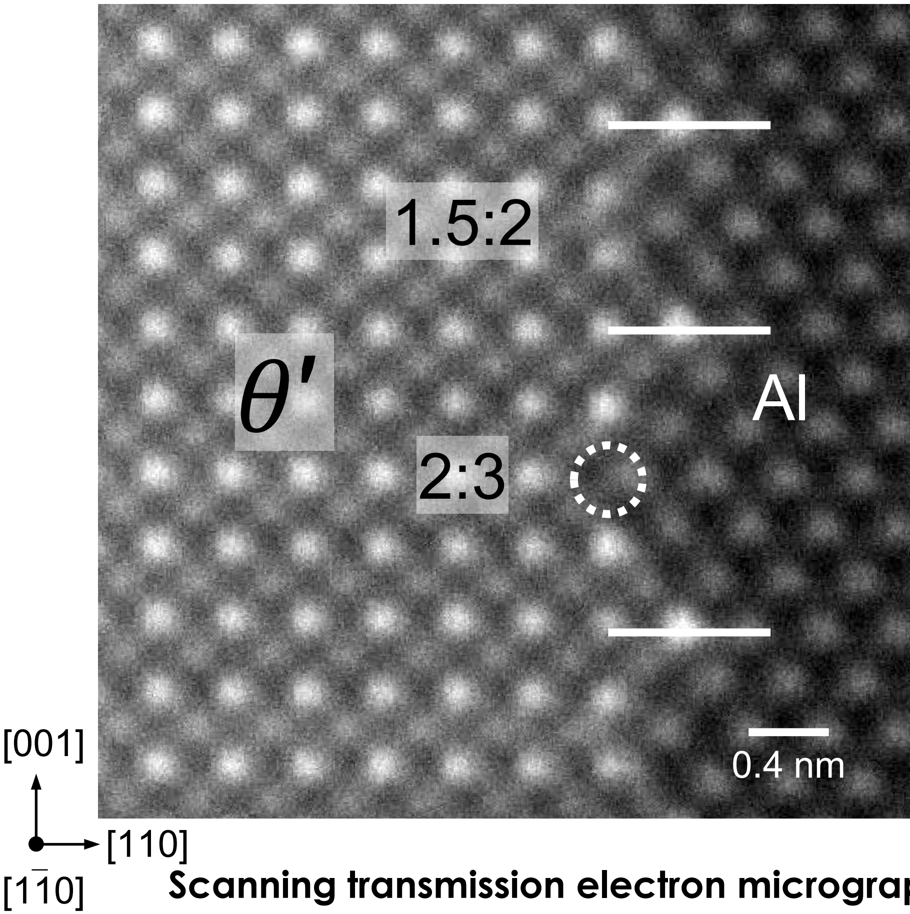


- Understanding interfaces and segregation to interfaces is key to developing the next generation precipitation strengthened alloys (e.g. for pistons)

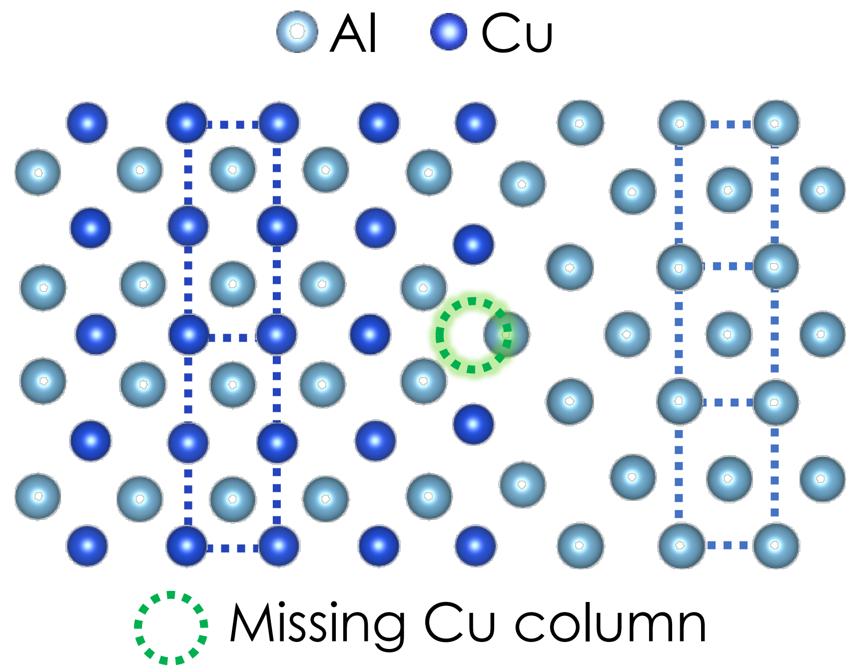
Advanced characterization guides atomistic calculations with high performance computing

 # Topic 1

Atomistic behavior of interfaces



Scanning transmission electron micrograph



Density Functional Theory model

- Overlooked interface between the Al matrix and key precipitate was modeled for further theoretical investigation. Modeling guided by advanced characterization.

Combine *in-situ* microscopy with calculations and predictions

- Define the conditions for critical phase transformations that lead to a degradation in mechanical properties

 # Topic 2

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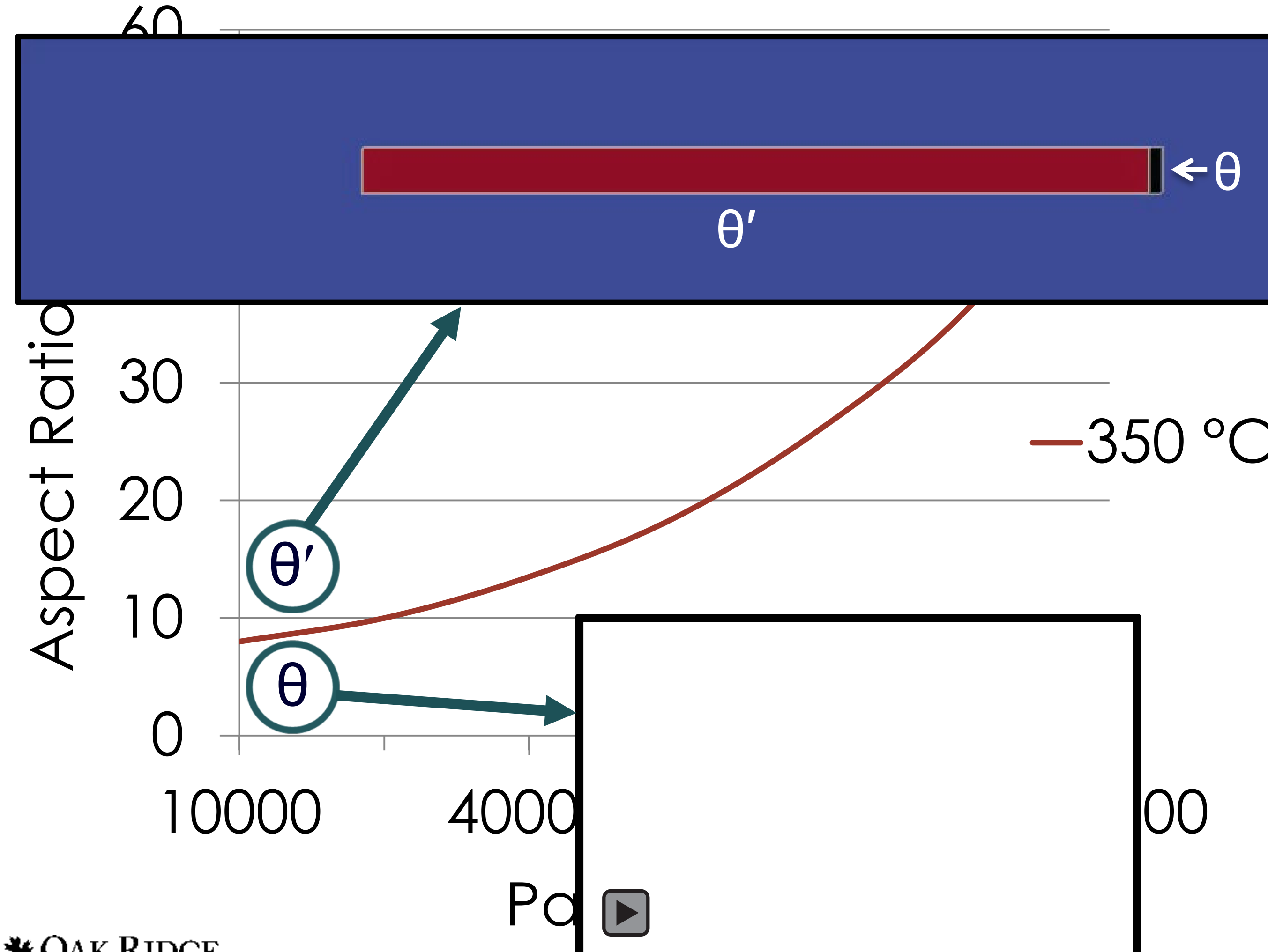
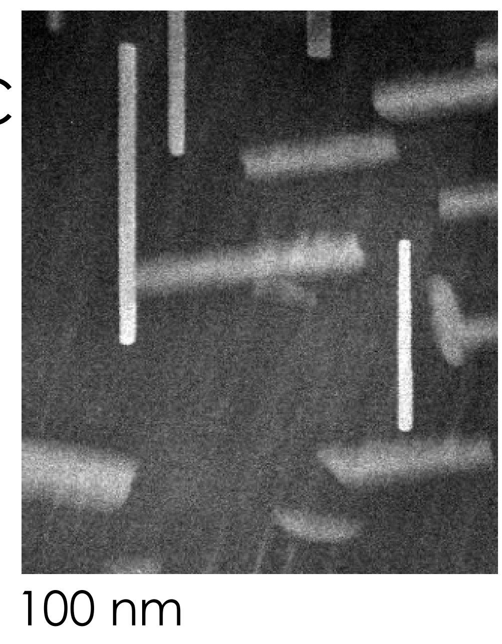
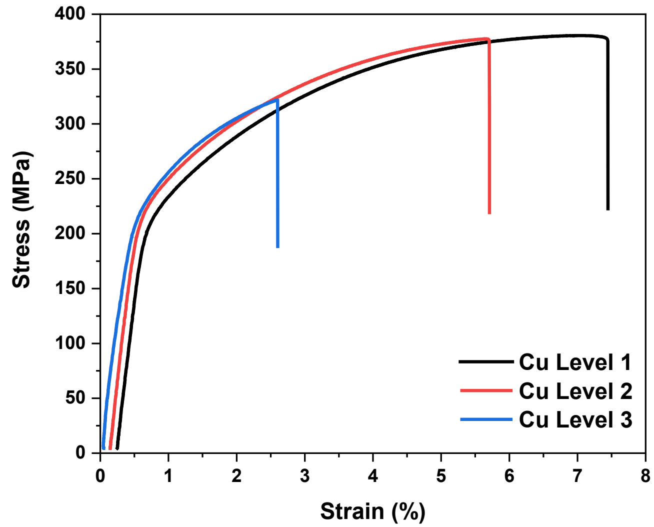


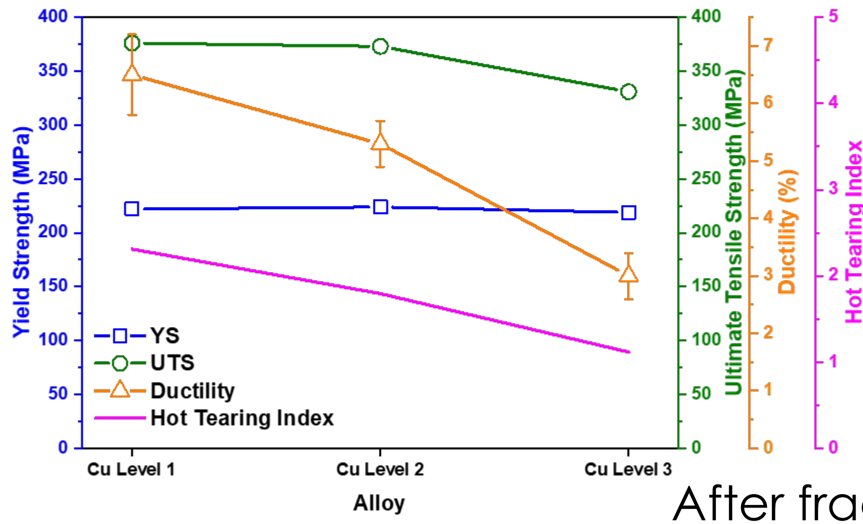


Development of microstructure-mechanical property relationships in ACMZ alloys for commercialization (different copper content affects grain boundary)

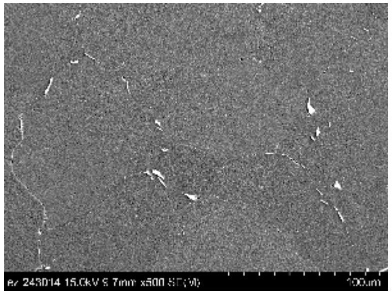
 # Topic 3

Mechanical Property Prediction





Finite element simulations with microstructures as input



After fracture

Multipoint constraint; Isotropic elasticity and plasticity

Responses to Previous Year Reviewer's Comments

- N/A

Collaboration and Coordination with Other Institutions

- Lead
  - Oak Ridge National Laboratory
- Partners
  - Pacific Northwest National Laboratory
  - Argonne National Laboratory
- Soliciting industry partners for Year 2 and beyond CRADAs (in Subtask 1B)

Remaining Challenges and Barriers

- Several gaps exist in ICME models; for example those pertaining to microstructural evolution and fatigue property prediction. These are barriers for future cast aluminum alloys for engine applications, in general.
- Commercialization barriers
  - Engine components can perform differently compared to laboratory scale castings. There are unknowns such as thermomechanical fatigue response, corrosion resistance, machinability and engine testing response of alloy before the alloys can be commercialized.
  - OEMs require a full materials card before they consider going into the design phase of a component
  - OEMs are needed to transition technology to their applications

Proposed Future Research

- Fundamental efforts will include
  - strategies implemented that improve the thermal stability of precipitates (to > 400°C)
  - alternative strategies will include dispersion hardening alloys
  - to establish the microstructure and mechanical property relationships of interest

- Applied efforts will include
  - improvement of intermediate temperature ductility and low cycle fatigue resistance of ACMZ alloys
  - generation of a thermomechanical property database for alloys of interest
  - Corrosion studies

Summary

- **Relevance:** Develop, using ICME, more robust engine materials that can withstand higher temperatures and combustion pressures, leading to further increases in power densities of engines.
- **Approach:** ICME approach used to accelerate the development of cast aluminum alloys.
- **Collaborations:** PNNL and ANL (three national labs are actively participating). Seeking CRADA partnerships in out-year.
- **Technical Accomplishments:**
  - Key activities in atomistic behavior of interfaces feeds the microstructural evolution models which in turn inform the mechanical property models.
  - New alloy concepts being developed and implemented based on fundamental studies
  - Thermomechanical data on a series of ACMZ alloy compositions generated for commercialization
- **Future Work:**
  - New alloys for next generation engines
  - Generation of thermomechanical data to support commercialization activities
  - Additive versions of aluminum alloys will be developed in a parallel activity (Thrust 3)